Ab initio translationally invariant nucleon-nucleus optical potentials

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I am presenting the work:

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Ab initio translationally invariant nucleon-nucleus optical potentials

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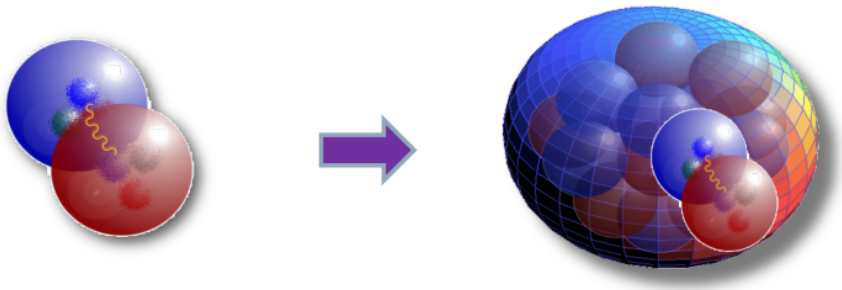
Outline

What do we mean by *ab initio*?

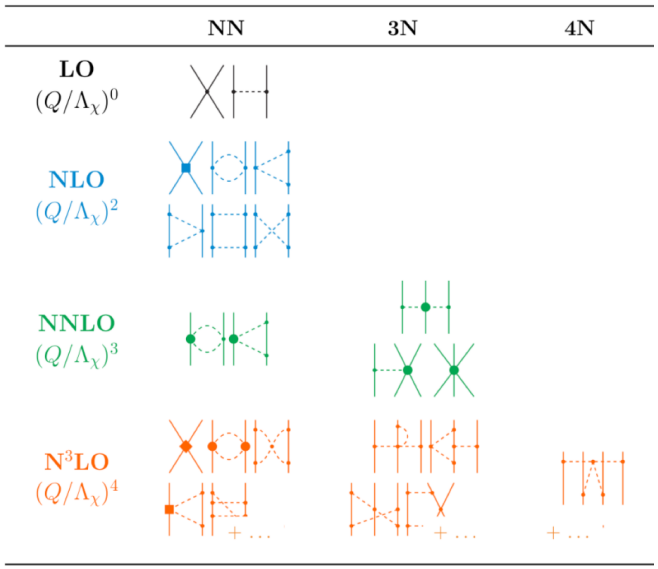
First Principles ***Many-body Dynamics***



- We part from *first principles* (QCD)
- We use this to solve the many-body problem.

A plethora of many-body methods:

- In-medium similarity renormalization group
- Coupled cluster method
- Self-consistent Green's functions
- Configuration interaction approaches
- Quantum Monte Carlo
- Lattice effective field theory



What is the specific problem we are trying to solve?

How do we get an optical potential from these *ab initio* interactions?

We use a self-consistent Green's function approach combined with the configuration interaction method of the Symmetry-adapted No-Core Shell Model, the so called: SA-NCSM/GF.

Green's function method

The time-ordered particle-hole Green's function, Fourier-transformed over the time component:

$$G(\mathbf{r},\mathbf{r}';E) = \lim_{\epsilon\to 0} \langle \Psi_0^A | \left[a_{\mathbf{r}} + a^\dagger_{\mathbf{r}'} \right] \times \frac{1}{E - (\hat{H} - E_0^A - i\epsilon)(\hat{N} - A)} \left[a_{\mathbf{r}} + a^\dagger_{\mathbf{r}'} \right] | \Psi_0^A \rangle$$

Two pieces of information:

- The numerator: transition amplitudes for addition and removal of nucleons.
- the denominator: excitation energies.

Green's function method

We can obtain a potential using Green's functions:

$$V^J_{J_0;\ell j\ell' j'}(r,r') = \sum_{nn'}^{n_{\max}} \left(E\delta_{nn'} - \langle n\ell | \hat{T}_{\rm rel} | n'\ell' \rangle \right) R_{n\ell}(r) R_{n'\ell}(r')$$
$$- \sum_{nn'}^{n_{\max}} \left(G^J_{J_0;n\ell j,n'\ell' j'} \right)^{-1} R_{n\ell}(r) R_{n'\ell'}(r'),$$

where

$$G^J_{J_0;n\ell j,n'\ell' j'}(E) = \langle \Phi^{J^+}_{J_0,n\ell j} | \frac{1}{E-(H-E^A_0)+i\epsilon} | \Phi^{J^+}_{J_0,n'\ell' j'} \rangle$$
$$\langle \Phi^{J^-}_{J_0,n;\ell' j'} | \frac{1}{E-(H-E^A_0)+i\epsilon} | \Phi^{J^-}_{J_0,n\ell j} \rangle \, ,$$

and also

$$|\Phi^{J^+}_{J_0,n\ell j}\rangle = (-)^{j+J_0-J} \left[a^\dagger_{n\ell j} \, |\Psi^A_{0,J_0}\rangle \right]^J$$
$$|\Phi^{J^-}_{J_0,n\ell j}\rangle = (-)^n (-)^{j+J_0-J} \left[\tilde{a}_{n\ell j} \, |\Psi^A_{0,J_0}\rangle \right]^J .$$

Removing the center of mass excitations

Long standing problem with Green's functions methods:

- Spurious center of mass contamination.

Generally neglected for heavier systems and valence space calculations. BUT...

$$G^{J}_{J_0;n\ell j,n'\ell' j'}(E) = \langle \Phi^{J^+}_{J_0,n\ell j} | \frac{1}{E-(H-E_0^A)+i\epsilon} | \Phi^{J^+}_{J_0,n'\ell' j'} \rangle$$
$$\langle \Phi^{J^-}_{J_0,n;\ell' j'} | \frac{1}{E-(H-E_0^A)+i\epsilon} | \Phi^{J^-}_{J_0,n\ell j} \rangle \, ,$$

both the $A+1$ and $A-1$ necessarily have CM motion.

Lawson method for Green's functions

The solution is the Lawson method.
Small reminder:

$$H + \lambda_{\mathrm{CM}} \hat{N}_{\mathrm{CM}}$$

The Green's functions in Lehman representation:

$$G^{J^+}_{ba(L)}(E) = \sum_{k\Gamma_k} \frac{\langle \Phi^{J^+}_a | \Psi^{A+1}_{k\Gamma_k} \rangle_{\mathrm{L}} \langle \Psi^{A+1}_{k\Gamma_k} | \Phi^{J^+}_b \rangle_{\mathrm{L}}}{E - (\epsilon^+_k + \lambda_{\mathrm{CM}} N^{\mathrm{CM}}_k) + i\epsilon}$$

$$G^{J^-}_{ab(L)}(E) = \sum_{k\Gamma_k} \frac{\langle \Phi^{J^-}_b | \Psi^{A-1}_{k\Gamma_k} \rangle_{\mathrm{L}} \langle \Psi^{A-1}_{k\Gamma_k} | \Phi^{J^-}_a \rangle_{\mathrm{L}}}{E - (\epsilon^-_k + \lambda_{\mathrm{CM}} N^{\mathrm{CM}}_k) - i\epsilon}$$

Nice equation but in practice not so straightforward! And also... what about spin coupling?

Lawson method for Green's functions

Some math later...

$$G^{J^\pm}_{ab(L)}(E) = \sum_{k\alpha\beta}\left[\sum_{\Gamma_k}\frac{\mathcal{M}^{\alpha\pm}_{a;\Gamma_i\Gamma_k}\mathcal{M}^{\beta\pm}_{b;\Gamma_i\Gamma_k}}{E-(\epsilon^\pm_k \pm \lambda_{\rm CM}N^{\rm CM}_k)\pm i\epsilon}\right]\langle\Phi^\pm_{i\alpha}|\Psi_k\rangle\langle\Psi_k|\Phi^\pm_{i\beta}\rangle\,,$$

where the $\mathcal{M}^{\alpha\pm}$ are related to Talmi-Moshinsky coefficients and spin coupling coefficient.

With $\Gamma = (N_{\rm CM}, L_{\rm CM}, M_{\rm CM})$ the only non-zero contribution is $\Gamma = (0,0,0)$.

$$\langle\Phi^\pm_{i\alpha}|\frac{1}{E-(\hat{H}-E^A_i-i\epsilon)(\hat{N}-A)}|\Phi^\pm_{i\beta}\rangle =$$
$$\frac{1}{\mathcal{M}^{\alpha\pm}_{\alpha;00}\mathcal{M}^{\beta\pm}_{\beta;00}}\langle\Phi^{0\pm}_{i0\alpha}|\frac{1}{E-(\hat{H}+\lambda_{\rm CM}\hat{N}_{\rm CM}-E^A_i-i\epsilon)(\hat{N}-A)}|\Phi^{0\pm}_{i0\beta}\rangle$$

Final expressions

For the regime $E > \varepsilon_F^+$:

$$G^{J-}_{\beta\alpha;E>\varepsilon_F^+} = \left(\frac{A+1}{A}\right)^{\frac{n_\alpha+n_\beta}{2}} \left[\text{p.v.}\,\langle\Phi^{J0-}_\beta|\hat{G}(E,\epsilon=0)|\Phi^{J0-}_\alpha\rangle + i\pi\sum_{k\Gamma_k}\langle\Phi^{J0-}_\beta|\Psi_{k\Gamma_k}\rangle_{\text{L}}\langle\Psi_{k\Gamma_k}|\Phi^{J0-}_\alpha\rangle_{\text{L}}\,\delta(E-\varepsilon^-_k)\right]$$

For the regime $E < \varepsilon_F^-$:

$$G^{J-}_{\beta\alpha;E<\varepsilon_F^-} = \lim_{\epsilon\to 0}\left(\frac{A}{A-1}\right)^{\frac{n_\alpha+n_\beta}{2}}\langle\Phi^{J0+}_\alpha|\hat{G}(E,\epsilon)|\Phi^{J0+}_\beta\rangle_{\text{L}}$$

One final step: the Lanczos method

Finally we solve with a Lanczos method

$$G^{J+}_{\alpha\beta(L)} = \sqrt{\langle \Phi^{J0+}_{\beta} | \Phi^{J0+}_{\beta} \rangle} \sum_k \langle \Phi^{J0+}_{\alpha} | q_k \rangle \langle q_k | \frac{1}{z - \hat{H}} | q^{\beta}_0 \rangle ,$$

with $z = E + E^A_0 + i\epsilon$ and the normalized pivots

$$|q^{\beta}_0\rangle = \frac{\Phi^{J0+}_{\beta}}{\sqrt{\langle \Phi^{J0+}_{\beta} | \Phi^{J0+}_{\beta} \rangle}}.$$

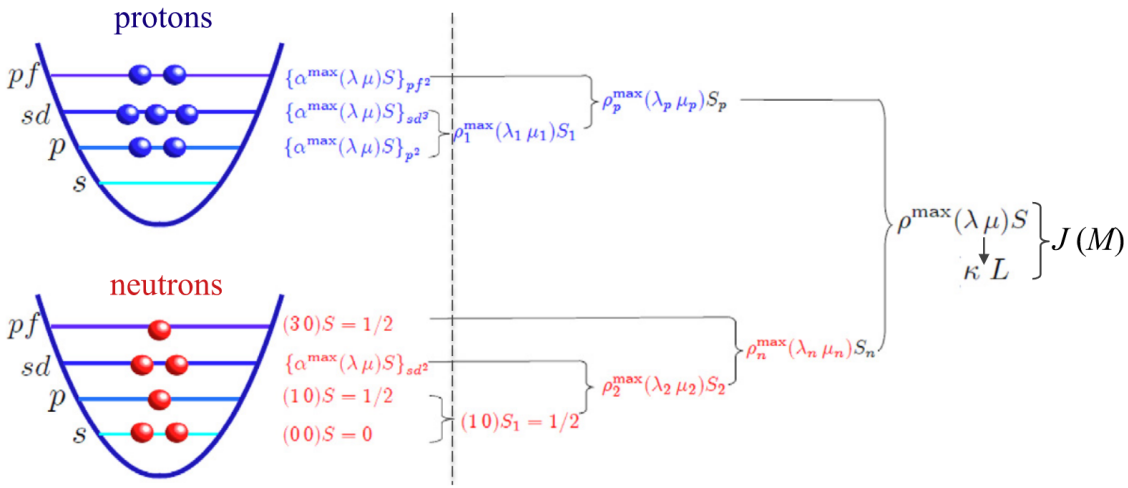
Symmetry-adapted no-core shell model

Configuration interaction many-body approach to the atomic nuclei

- shell model $\rightarrow$ valence particles in shells.
- no-core $\rightarrow$ no frozen core, all particles active.
- symmetry-adapted $\rightarrow$ basis selected with symmetries in mind.

Summarized features of the SA-NCSM:

- SU(3)-coupled basis states or Sp(3,R)-coupled basis states.
- The selected model space consists of physically relevant basis states + exact center of mass factorization.



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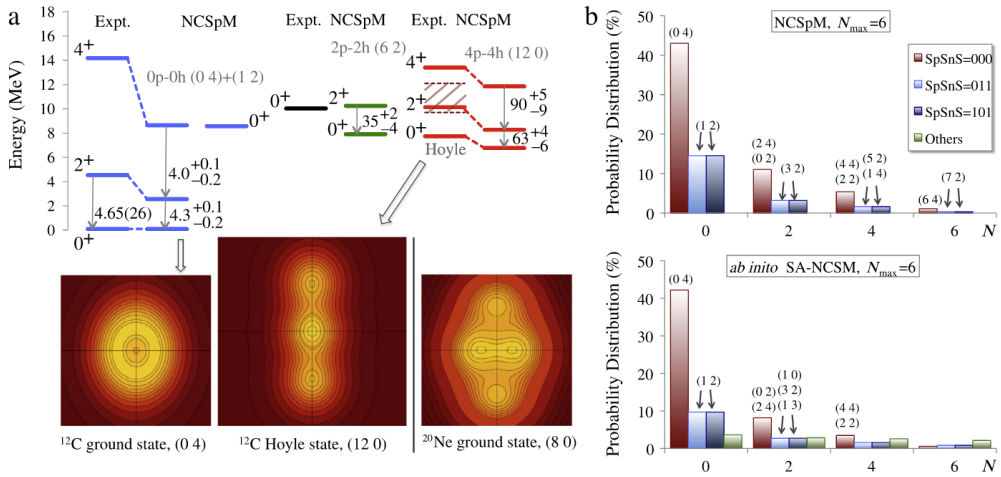

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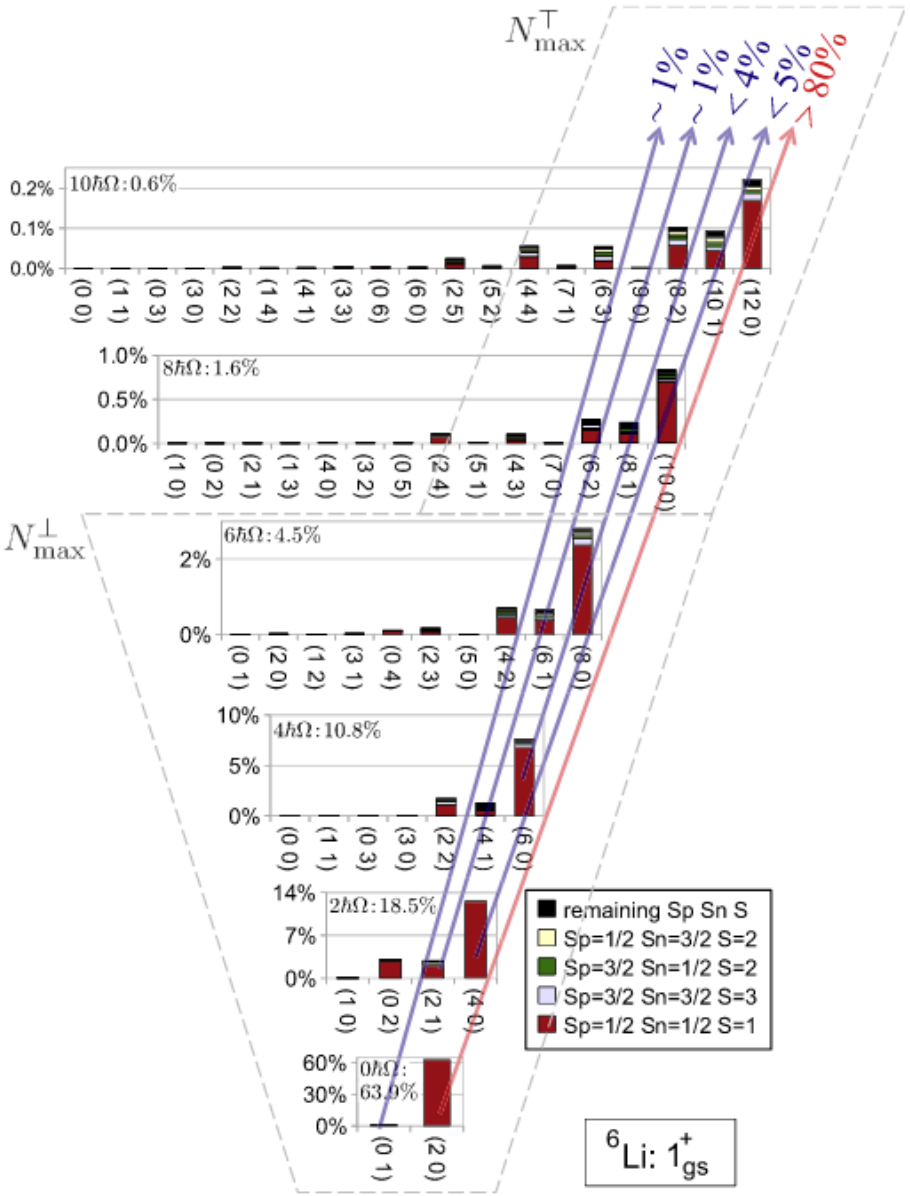
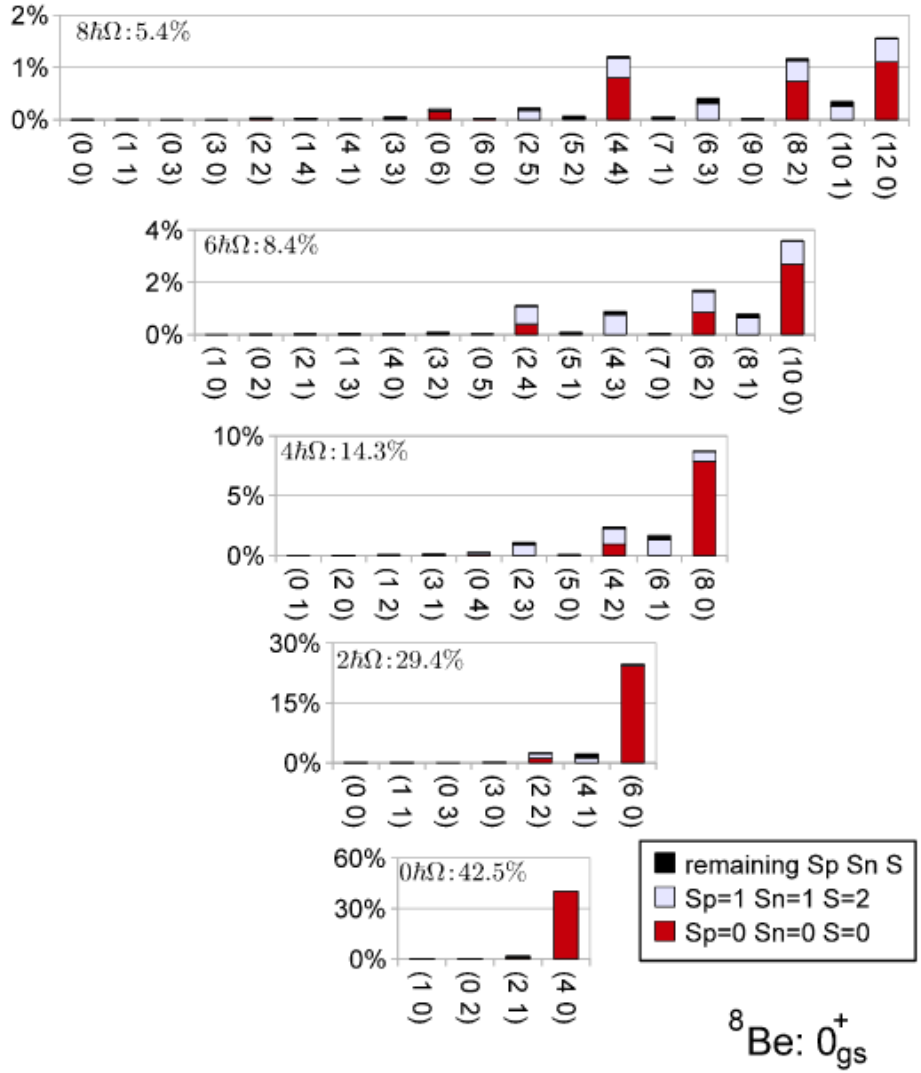




Application of the Green's function method

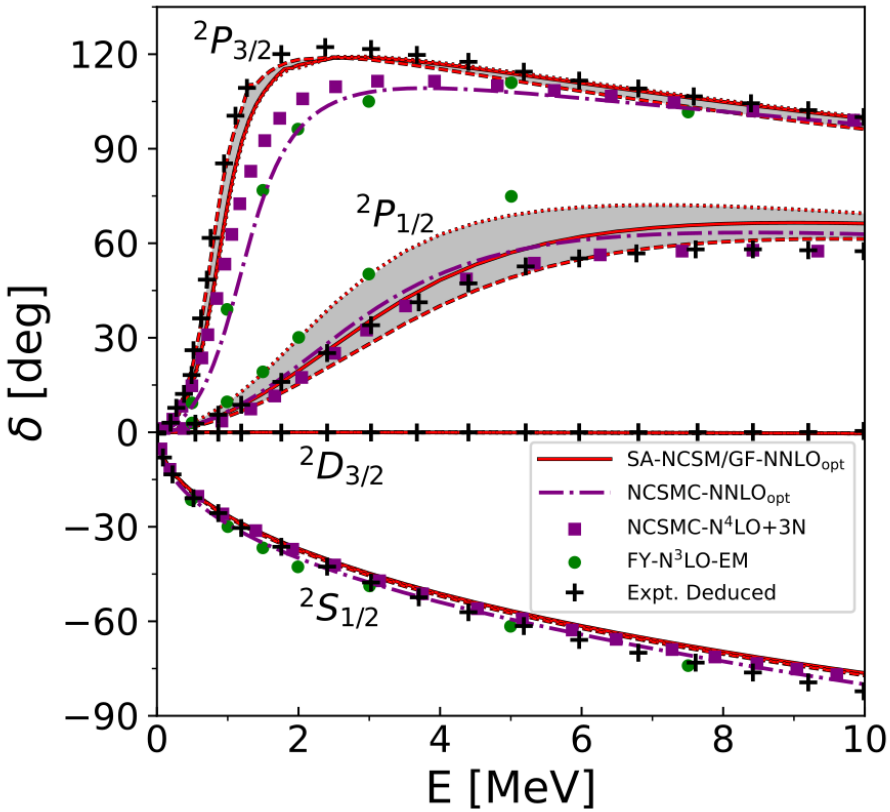
This method was applied to the ^{4}He(n, n) elastic scattering.
Calcultated with SA-NCSM using the $\mathrm{NNLO_{opt}}$ chiral potential:

- ^{4}He ground state,
- $A+1$ and $A-1$ systems (used in the Lanczos).

Important parameters:

- $\hbar\omega = 12 - 20$ MeV,
- $N_{\max} = 13$,
- $\lambda_{\mathrm{CM}} = 100$.

Phase shifts



- Computed with R-matrix code.
- Good agreement with the experimental phase shifts.
- At $\hbar\omega = 16$, threshold within 230 keV from experiment.

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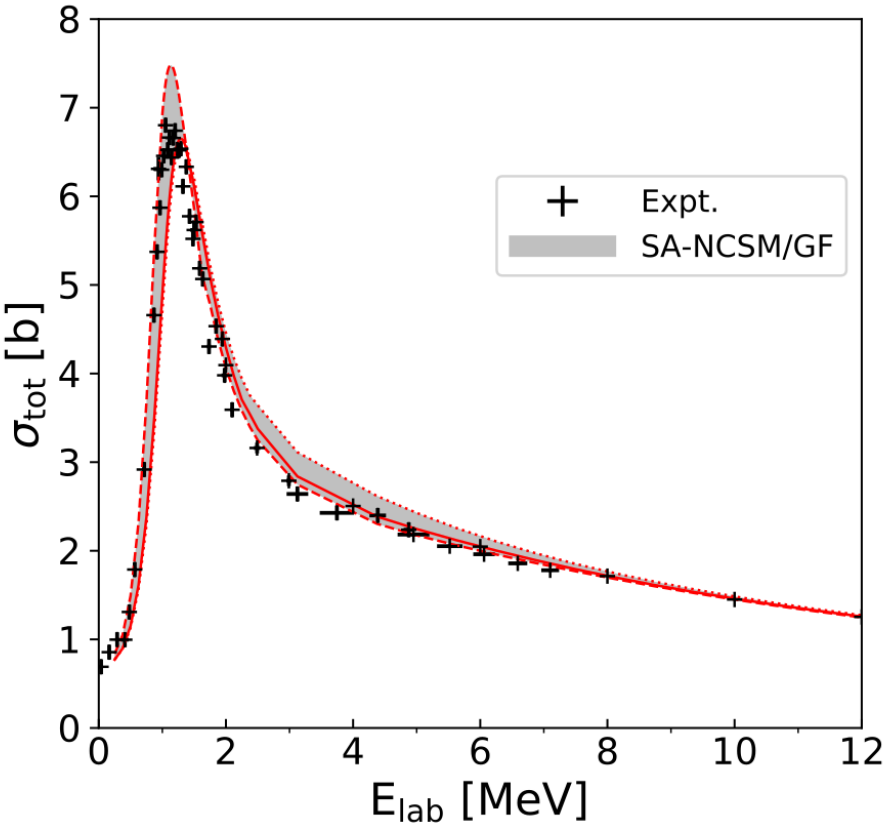
Cross-section



- From phase shifts to cross-section.
- In excellent agreement with the experiment.

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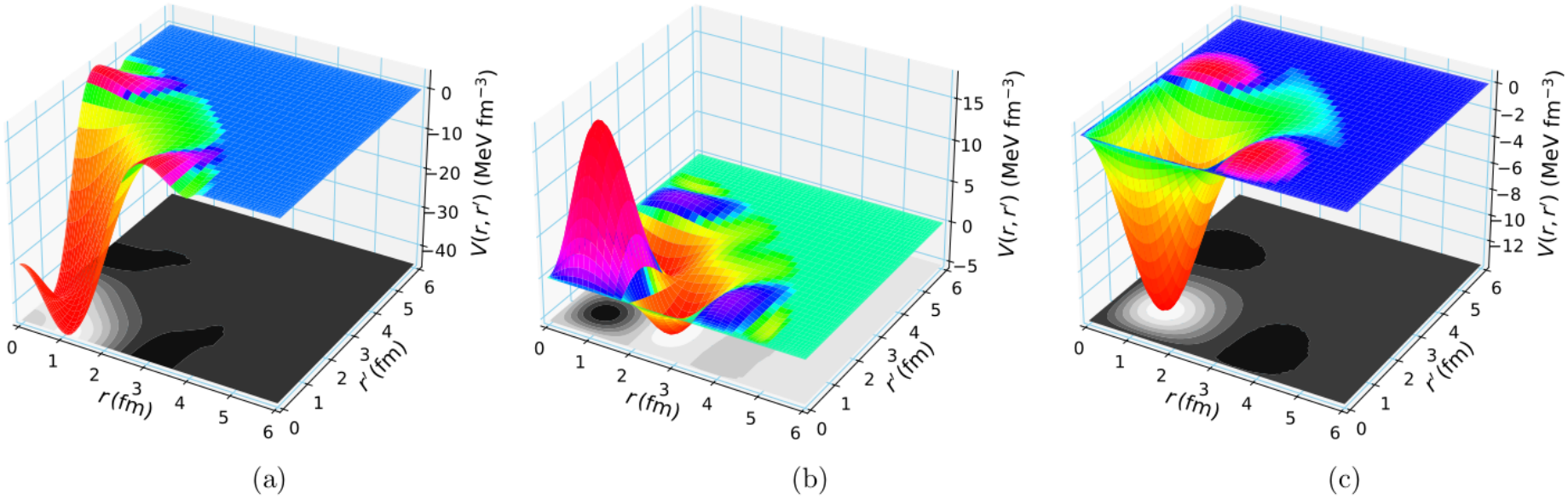
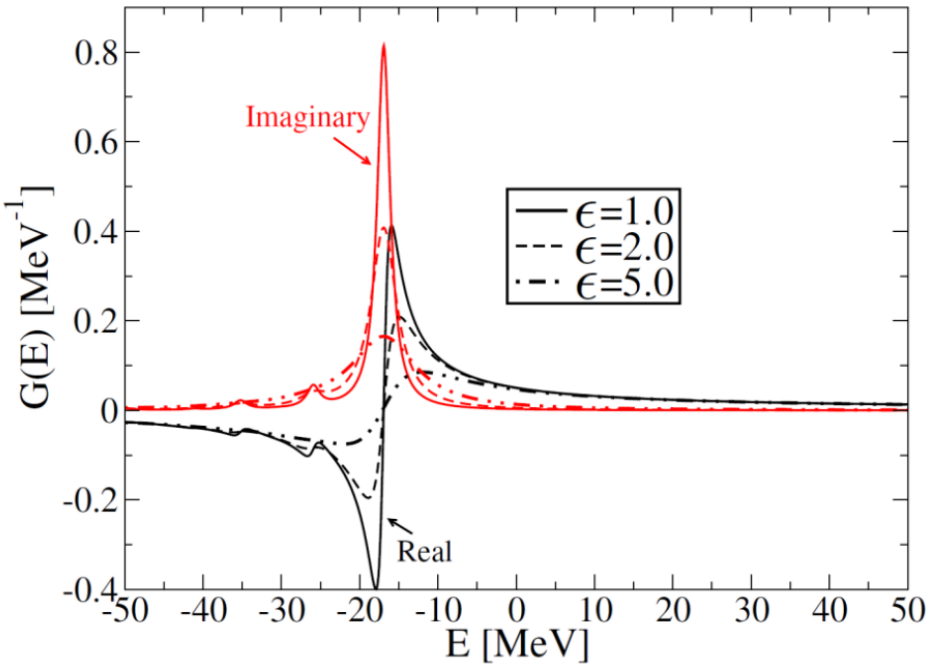
Some comments about the optical potential



M Burrows et al., PRC **109**, 014616 (2024) (a) $s_{1/2}$ (b) $p_{1/2}$ (c) $p_{3/2}$

- Potential remains largely non-local
- Very similar shapes to NCSM-RGM and NCSMC potentials?

Spectral functions



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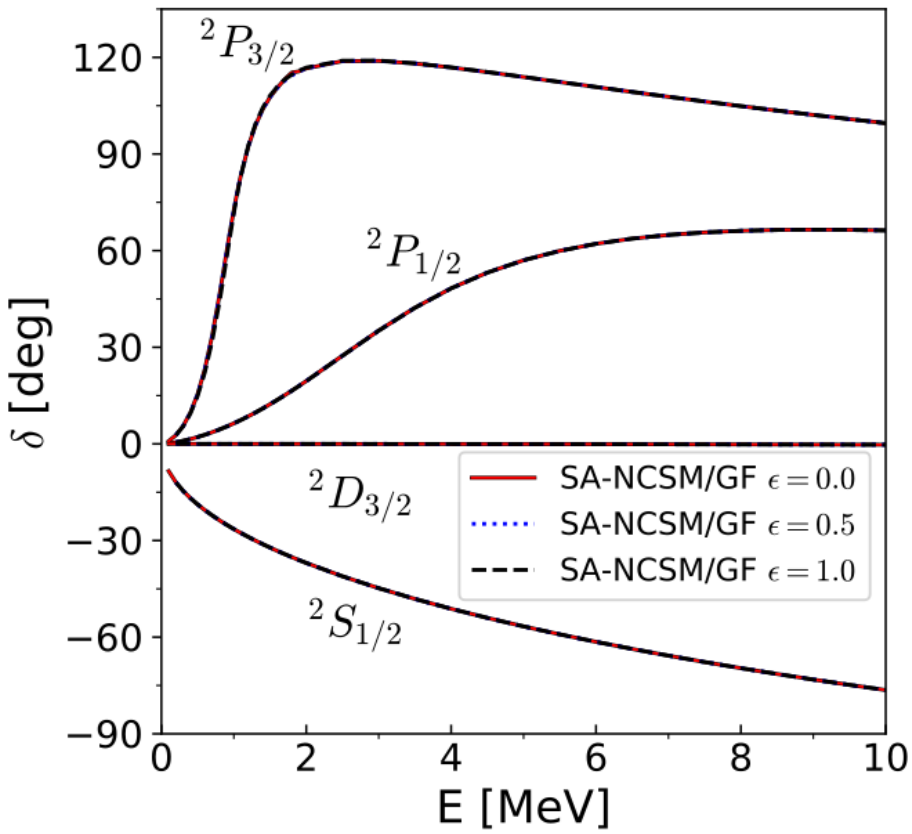
- ^{3}He energies clearly visible.
- If we are far from this energy regime, calculations should not depend on ϵ.

About the dependence of parameters: ϵ



- Practically no dependence of ϵ

$$G^{J}_{J_0;n\ell j,n'\ell' j'}(E) = \langle \Phi^{J^+}_{J_0,n\ell j} | \frac{1}{E-(H-E_0^A)+i\epsilon} | \Phi^{J^+}_{J_0,n'\ell' j'} \rangle$$
$$\langle \Phi^{J^-}_{J_0,n;\ell' j'} | \frac{1}{E-(H-E_0^A)+i\epsilon} | \Phi^{J^-}_{J_0,n\ell j} \rangle \, .$$

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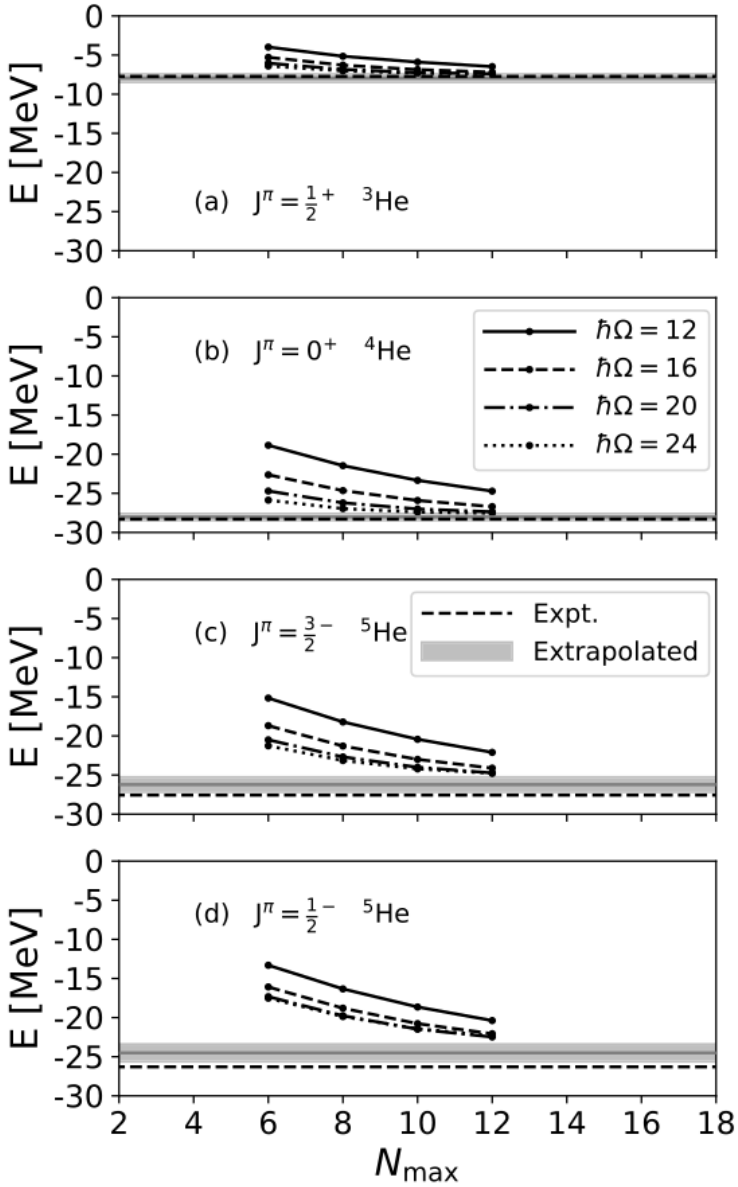
About the dependence of parameters: $N_{\max}$



- Converging trend with $N_{\max}$.
- Ground state energy obtained with Shank's approximation.

Small reminder:

- ^{3}He and ^{5}He excited states are important because they are poles of the Green's functions!

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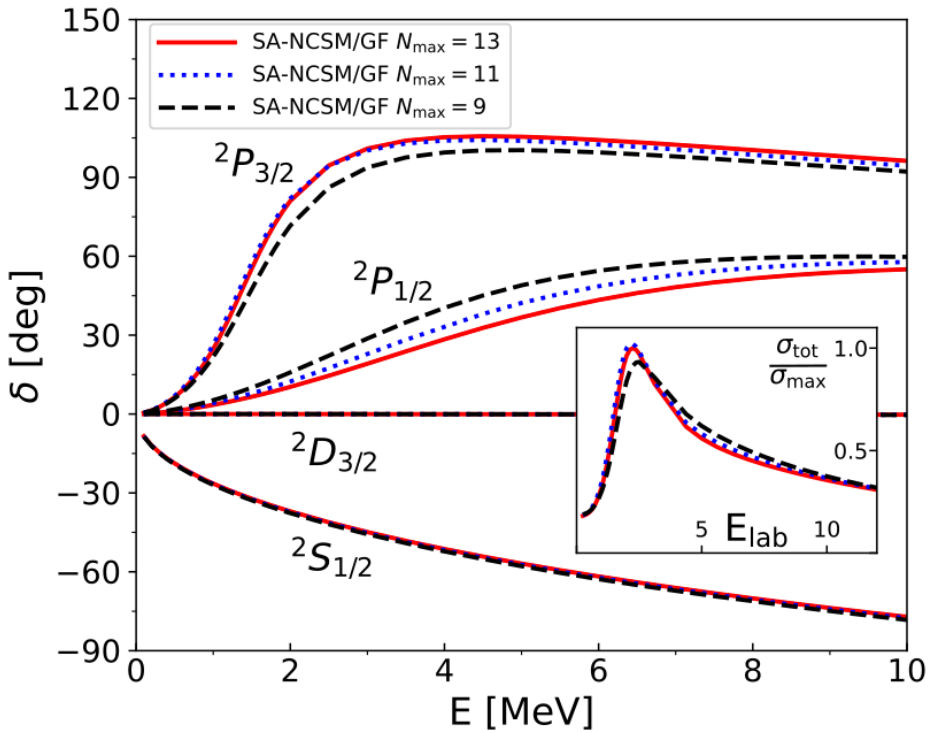
About the dependence of parameters: $N_{\max}$



Let's not forget to check the reaction observables too!

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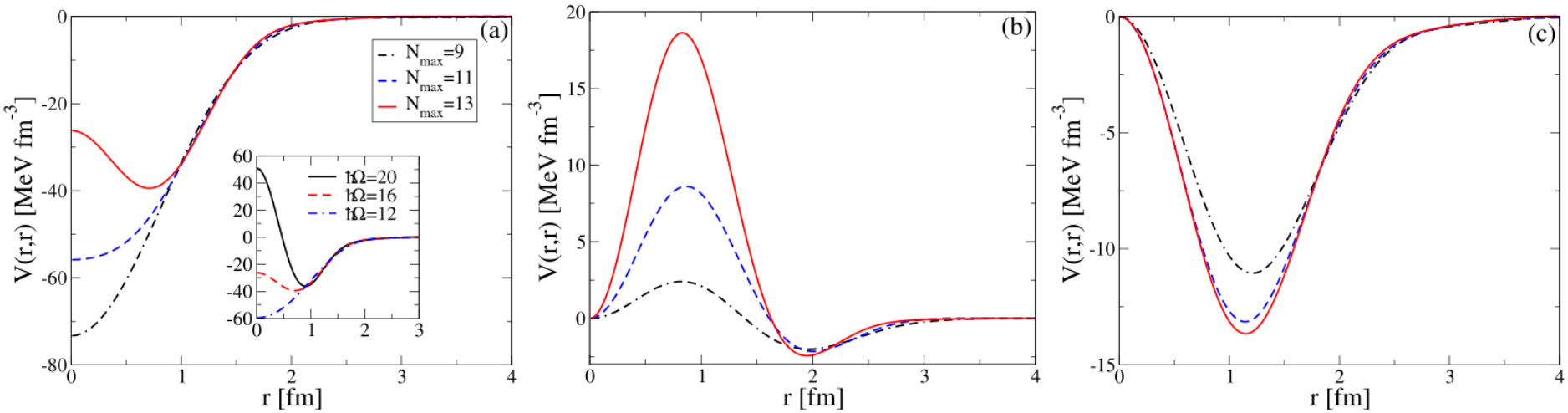
Is everything okay in the non-local potentials?



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(a) $s_{1/2}$ (b) $p_{1/2}$ (c) $p_{3/2}$

The diagonal of the non-local potentials do not seem to converge...

however...

Non-local potentials are not observables! Let's try to extract some physics from this:

- Higher $N_{\max}$, $\hbar\omega$ leads to a more repulsive core.
- The disagreement is only in the interior region, which is accessible at higher energies!

Conclusion

- The SA-NCSM/GF was developed to construct the first *ab initio* translationally invariant optical potentials for the ^{4}He + n system.
- The spurious center of mass excitations have been removed using the Lawson method.
- Although computationally intensive, it is possible to do this calculations using the Lanczos algorithm.

Outlook:

- Proton and neutron elastic scattering on heavier nuclei, e.i. ^{6}He, ^{12}C, ^{16}O, ^{40}Ca, etc.
- Generalization to $d - A$ potentials and inelastic scattering.

Back up

Cramer's rule

To calculate the matrix elements,

$$x^{\beta}_{k0} \equiv \left\langle q_k \left| \frac{1}{z-\hat{H}} \right| q^{\beta}_0 \right\rangle = x^{\beta}_{0k}, \tag{38}$$

the continued fraction evaluation, based on Cramer's rule [55], is used:

$$\begin{aligned} x_{0k} &= \frac{1}{(z-a_k)\lambda_{0k-1} - b_k\lambda_{0k-2} + \lambda_{0k-1}g_{k+1}}, \\ \lambda_{0k} &= \frac{(z-a_k)\lambda_{0k-1} - b_k\lambda_{0k-2}}{b_{k+1}}, \\ g_k &= \frac{-b_k^2}{(z-a_k) - \dfrac{b_{k+1}^2}{(z-a_{k+1}) - \dfrac{b_{k+2}^2}{\cdots}}}, \end{aligned} \tag{39}$$

Orthonormalization

- Solve for J_0 G.S.
- Generate cluster basis states.
- ensure $\mathcal{N}^p_{ab}(L) + \mathcal{N}^h_{ba}(L) = \delta_{ab}$

earlier study [54]. This is achieved by applying a projection operator $\hat{\mathcal{P}}_0$, such that $|\Phi_a^{J0\pm}\rangle_{\rm L} = \hat{\mathcal{P}}_0 |\Phi_a^{J\pm}\rangle_{\rm L}$, where

$$\hat{\mathcal{P}}_0 = \prod_{N^{\rm CM}=1}^{N_{\rm max}} \left(\mathbb{1} - \frac{\hat{N}_{\rm CM}}{N^{\rm CM}} \right). \tag{34}$$

The $|\Phi_a^{J0\pm}\rangle_{\rm L}$ cluster basis states are then used to calculate $\langle \Phi_a^{J0\pm} | \hat{\tilde{G}}(E, \epsilon) | \Phi_b^{J0\pm} \rangle_{\rm L}$ matrix elements for the t.i. Green's